# Bromoacetic acid, 2-naphthyl ester

**Inchi:** InChI=1S/C12H9BrO2/c13-8-12(14)15-11-6-5-9-3-1-2-4-10(9)7-11/h1-7H,8H2
**InchiKey:** XJWDIZWNDCUOMG-UHFFFAOYSA-N
**Formula:** C12H9BrO2
**SMILES:** O=C(CBr)Oc1ccc2ccccc2c1
**Mol. weight [g/mol]:** 265.10

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 39.99 | kJ/mol | Joback Method |
| hf | -93.35 | kJ/mol | Joback Method |
| hfus | 25.58 | kJ/mol | Joback Method |
| hvap | 62.48 | kJ/mol | Joback Method |
| log10ws | -4.02 | | Crippen Method |
| logp | 3.140 | | Crippen Method |
| mcvol | 161.660 | ml/mol | McGowan Method |
| pc | 3484.76 | kPa | Joback Method |
| rinpol | 1890.00 | | NIST Webbook |
| rinpol | 1890.00 | | NIST Webbook |
| tb | 667.05 | K | Joback Method |
| tc | 914.19 | K | Joback Method |
| tf | 428.60 | K | Joback Method |
| vc | 0.608 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 370.47 | J/mol×K | 667.05 | Joback Method |
| cpg | 382.23 | J/mol×K | 708.24 | Joback Method |
| cpg | 393.04 | J/mol×K | 749.43 | Joback Method |
| cpg | 402.97 | J/mol×K | 790.62 | Joback Method |
| cpg | 412.09 | J/mol×K | 831.81 | Joback Method |
| cpg | 420.49 | J/mol×K | 873.00 | Joback Method |
| cpg | 428.25 | J/mol×K | 914.19 | Joback Method |
| dvisc | 0.0013275 | Pa×s | 428.60 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0009336 | Pa×s | 468.34 | Joback Method |
| dvisc | 0.0006937 | Pa×s | 508.08 | Joback Method |
| dvisc | 0.0005382 | Pa×s | 547.83 | Joback Method |
| dvisc | 0.0004321 | Pa×s | 587.57 | Joback Method |
| dvisc | 0.0003567 | Pa×s | 627.31 | Joback Method |
| dvisc | 0.0003013 | Pa×s | 667.05 | Joback Method |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U308052&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |